1,10-Phenanthroline, 2,9-dimethyl-

Other names:	2,9-Dimethyl-o-phenanthroline
	2,9-Dimethylphenanthroline
	2,9-dimethyl-1,10-phenanthroline
	Neo-Cuproin
	neocuproine
Inchi:	InChI=1S/C14H12N2/c1-9-3-5-11-7-8-12-6-4-10(2)16-14(12)13(11)15-9/h3-8H,1-2H3
InchiKey:	IYRGXJIJGHOCFS-UHFFFAOYSA-N
Formula:	C14H12N2
SMILES:	Cc1ccc2ccc3ccc(C)nc3c2n1
Mol. weight [g/mol]:	208.26

Physical Properties

Property code	Value	Unit	Source
af	0.5330		Cheméo Relay (1.0)
hf	228.93	kJ/mol	Cheméo Relay (1.0)
hfus	17.60	kJ/mol	Heat capacities and molar enthalpies and entropies of fusion for anhydrous 1,10-phenanthroline and 2,9-dimethyl-1,10-phenanthroline
hvap	87.97	kJ/mol	Cheméo Relay (1.0)
ie	7.94	eV	Cheméo Relay (1.0)
log10ws	-3.18		Cheméo Relay (1.0)
logp	3.400		Crippen Method
mcvol	165.400	ml/mol	McGowan Method
pc	3347.82	kPa	Cheméo Relay (1.0, beta)
tb	628.46	K	Cheméo Relay (1.0)
tc	918.16	K	Cheméo Relay (1.0)
tf	444.61	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	17.60	kJ/mol	435.90	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C484117&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Heat capacities and molar enthalpies and entropies of fusion for anhydrous 1,10-phenanthroline and 2,9-dimethyl-1,10-phenanthroline:	https://www.doi.org/10.1016/j.tca.2007.10.001

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point